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Polarity and structure of P(X)-modified (X = O, S) arylcarbamoylmethylphosphine oxides and sulfides

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Abstract

© 2016, Pleiades Publishing, Ltd.As shown by the dipole moment method and quantum chemical calculations, (arylcarbamoylmethyl) diphenylphosphine oxides and sulfides exist as equilibrium mixtures of several rotational isomers stabilized by H · · · X intramolecular hydrogen bonds (X = O, S). The most energetically favorable rotamer and its fraction have been determined for each compound.

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